

Ecosystem Predictions with Approximate vs. Exact Light Fields

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LONG-TERM GOAL

The overall goal of this work is to develop an extremely fast but accurate radiative transfer model, called EcoLight, for use in coupled physical-biological-optical ecosystem models, and then to demonstrate the ecological necessity and computational feasibility of including accurate light field predictions in coupled physical-biological-optical ecosystem models.

OBJECTIVES

Currently available ecosystem models often use fairly sophisticated treatments of the physics (e.g., advection and upper-ocean thermodynamics and mixing) and biology (e.g., primary production, nutrient utilization, and grazing) but use grossly oversimplified treatments of the optics. The optics component of coupled ecosystem models is sometimes just a single equation parameterizing the scalar irradiance in terms of the chlorophyll concentration and a few parameters such as the solar zenith angle. Such simple models often fail even in Case 1 waters, and they can be wrong by orders of magnitude in Case 2 or optically shallow waters. The objective of this work was develop a radiative transfer model that can be used in coupled models to bring the optics component up to the level of accuracy and sophistication needed for ecosystem models that are being applied to any water body, including Case 2 and optically shallow waters.

APPROACH

The Hydrolight radiative transfer model (Mobley et al., 1993; Mobley 1994; www.hydrolight.info) provides an accurate solution of the radiative transfer equation (RTE) for any water body, given the absorption and scattering properties of the water body and boundary conditions such as incident sky radiance and bottom reflectance. However, the standard version of Hydrolight requires far too much computer time to make it suitable for use in ecosystem models where the light field must be computed at many grid points and at time intervals of order one hour. However, ecosystem models require only the scalar irradiance as a function of depth and wavelength, $E_o(z, \lambda)$, which makes it possible to solve an azimuthally averaged version of the radiative transfer equation (RTE), from which the irradiances can be obtained. Solving the azimuthally integrated RTE removes much of the computation load in Hydrolight, which solves for azimuthally dependent radiances.

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WORK COMPLETED

The core HydroLight code was reformulated to solve the azimuthally averaged RTE, and the new code, called EcoLight, was coded as a subroutine that can be incorporated into coupled ecosystem models. The EcoLight subroutine was then imbedded in an idealized physical-biological-optical ecosystem model called BioToys. The BioToys ecosystem model uses the ROMS physical model, the EcoSim biological model and, in its default mode, a simple analytical model for the scalar irradiance. The EcoSim analytical irradiance model was replaced by EcoLight for the comparisons presented here.

The ROMS physical model (Regional Ocean Modeling System; Shchepetkin and McWilliams, 2005; www.myroms.org) is a curvilinear-coordinate (terrain-following), free-surface, primitive equation model designed for prediction of physical oceanography quantities in coastal waters. The BioToys code uses a 6x6 horizontal grid version of ROMS 2.0 with periodic lateral boundary conditions. This spatially limited “generic” ROMS version was chosen to minimize run times during the EcoLight code development and verification simulations. For the simulations presented here, the grid is centered off the eastern United and has a horizontal grid resolution of approximately 13 km. The vertical grid has 30 points covering the upper 210 m of the water column; the vertical resolution ranges from approximately 2 m near the sea surface to 15 m at depth.

The EcoSim biological model (Ecosystem Simulation; Bissett et al., 1999a, 1999b, 2004) was developed for simulations of carbon cycling and biological productivity in Case 1 oceanic waters. This model includes four phytoplankton functional groups defined according to their pigment suites (small diatoms, large diatoms, dinoflagellates, and *synechococcus*). Each functional group has a unique set of accessory pigments, which varies with the group carbon-to-chlorophyll *a* ratio, $C:Chl_a$. Pigment packaging and accessory pigment concentration are functions of the chlorophyll *a* concentration within each functional group. The chlorophyll *a* content and other properties of each functional group evolve with the light history and nutrient status of the group. The model also includes components describing dissolved and particulate organic and matter, bacteria, and detritus. The interactions between these components describe autotrophic growth of and competition between the four phytoplankton groups, differential (non-Redfield ratio) carbon and nitrogen cycling, nitrification, grazing, and air-sea exchange of CO₂. The initial application of EcoSim to predictions of seasonal cycles of carbon cycling and phytoplankton dynamics in the Sargasso Sea showed that its predictions were consistent with measurement of various biological and chemical quantities at the Bermuda Atlantic Time-series Study station (Bissett et al., 1999a).

The absorption spectra of the phytoplankton functional groups change with light and nutrient adaptation. The four groups therefore respond differently to various wavelengths of the available light, and each particular group responds differently over time. EcoSim thus requires spectral irradiances at 5 nm bandwidths between 400 and 700 nm in order to model the changes within each functional group and competition between them. BioToys uses EcoSim version 2.0 (Bissett et al., 2004).

EcoSim Analytical Optics. The original EcoSim code uses the input sky spectral irradiance (obtained from an ancillary sky model, measurement, or climatology) to compute spectral downwelling plane irradiances just beneath the sea surface. These spectral downwelling plane irradiances are then propagated to depth using $E_d(z, \lambda) = E_d(0, \lambda) \exp[-\int_0^z K_d(z', \lambda) dz']$ and a simple model for K_d : $K_d(z, \lambda) = [a(z, \lambda) + b_b(z, \lambda)] / \mu_d(z, \lambda)$. Here $a(z, \lambda)$ is the total absorption coefficient (the sum of absorption by pure water and the various particulate and dissolved components), and $b_b(z, \lambda)$ is the total backscatter

coefficient. The phytoplankton absorption is obtained from the concentrations of the functional groups and their chlorophyll-specific absorption spectra. The backscatter and total scatter coefficients are obtained from chlorophyll-dependent models for Case 1 waters, using the total Chl_a concentration. The mean cosine for downwelling irradiance, $\mu_d(z, \lambda)$, is itself modeled by a simple function that merges estimates of the near-surface and asymptotic-depth mean cosines (Bisett et al., 1999b, Eqs. 18-22). Finally, the needed scalar irradiance $E_o(z, \lambda)$ is obtained from the computed $E_d(z, \lambda)$ and the approximation $E_o(z, \lambda) = E_d(z, \lambda)K_d(z, \lambda)/a(z, \lambda)$.

The biology is updated at each ROMS time step and grid point using the analytic formulas for the scalar irradiance just described. However, the irradiances computed within EcoSim do not feed back to the ROMS code which, for programming simplicity when merging the codes, retains its original short and long-wave light parameterization for mixed-layer heating calculations. Thus the physical model influences the biology via temperature and mixing, but the optical model employed within EcoSim does not influence the physical model. This simplification was made in these initial studies to avoid alterations to the ROMS code.

The EcoLight Optical Model. As stated above, EcoLight solves the azimuthally averaged RTE to obtain irradiances with the same accuracy at HydroLight. The inputs for EcoLight are the same as for HydroLight, namely the inherent optical properties (IOPs) of the water body, the incident sky radiance, and the bottom reflectance (in finite-depth waters). Unlike simple analytical light models, EcoLight can account for the effects of shallow bottoms and is valid for Case 2 waters. EcoLight also computes related quantities such as the nadir-viewing remote-sensing reflectance and diffuse attenuation functions corresponding to the bio-optical state of the ecosystem. This allows for validation of ecosystem model predictions using satellite ocean color radiometry, without an intervening step to convert a satellite-measured radiance to a chlorophyll concentration via an imperfect chlorophyll algorithm.

EcoLight takes the following philosophy. It is necessary to solve the RTE in order to incorporate the effects of the surface boundary conditions and to account for all IOP effects. However, once an accurate value of the scalar irradiance $E_o(z, \lambda)$ has been computed to some depth z_o deep enough to be free of surface boundary effects, it is not necessary to continue solving the RTE to greater depths, which is computationally expensive. As shown below, in many cases of practical interest, it is possible to extrapolate the accurately computed upper-water-column irradiances to greater depths and still obtain irradiances that are acceptably accurate for ecosystem predictions. Likewise, it is not necessary to solve the RTE at every wavelength in order to obtain acceptably accurate irradiances at the needed wavelength resolution. Omitting every other wavelength, for example, cuts the run time by one half. It is certainly not necessary to update the light field at every time step of the physical model (9 minutes in the simulations below).

EcoLight was packaged as a subroutine that allows it to be called from within an ecosystem model whenever updated values of $E_o(z, \lambda)$ are needed. That subroutine is used within BioToys to replace the analytic irradiance computations described above. The EcoLight subroutine takes the component concentration profiles generated by EcoSim, converts the concentrations to absorption, scattering, and backscattering coefficients according to the current pigment suites, generates scattering phase functions having the proper backscatter fraction, and uses those IOPs along with sky conditions and other input passed down from ROMS-EcoSim to compute the scalar irradiance as a function of depth and wavelength.

Two book chapters related to this work were published: Bissett et al. (2008) and Smith and Mobley (2008).

RESULTS

We first used BioToys with its original analytic irradiance model to perform an idealized five-year ecosystem simulation. The initial conditions were typical depth profiles of concentrations of the four phytoplankton functional groups and nutrients (NO_3 , NH_4 , PO_4 , etc.). The external physical forcing was based on daily measurements of solar irradiance and winds. The physical forcing depended on the day of the year but the daily cycle was the same for each year of the five-year simulation. The irradiances were recomputed *de novo* at every ROMS time step (9 minutes) and every grid point in the 6x6 spatial grid. The spectral scalar irradiance was computed at 5 nm resolution from 400 to 700 nm, and to a depth where the irradiance was a fraction $F = 0.001$ (0.1%) of the surface value. This run was the baseline for comparison with other run options.

We then ran BioToys with the analytic irradiances being recomputed only every hour (after the first computation after sunrise each day) and at only one grid point of the spatial grid. The irradiances at the uncomputed times and grid points were obtained by scaling the most recently computed values by the incident solar irradiance at the current time and location. The black and purple curves in Fig. 1 show that recomputing the irradiances hourly at only one grid point makes less than a 2% difference in the computed total chlorophyll values after 5 years of ecosystem development, compared to the baseline run. Therefore, for computation efficiency, we take the 1 hour (1HR), 1 grid point (1GP) frequency of recomputing the analytic irradiances as the baseline for subsequent EcoLight runs.

We then replaced the EcoSim analytic irradiance model with calls to EcoLight. The blue curve in Fig. 1 shows the resulting chlorophyll values during simulation year 5, for the same time, space, and wavelength resolution as the 1HR, 1GP run with the analytical irradiance model. This is the baseline for subsequent EcoLight runs. We see that, depending on the time of year, there are differences as large as a factor of two in the total Chl values, and the time of the spring bloom is delayed by roughly a month.

Figure 1 is sufficient to show that ***accurately computed irradiances give significantly different ecosystem development compared to approximate analytic irradiances, even in idealized Case 1 waters.***

However, the EcoLight run in Fig. 1 took 3.22 times as long as the run using the analytic irradiance model. (This is the total run time including the ROMS and EcoSim calculations, not just the irradiance calculations.) We therefore considered various optimizations for running EcoLight to reduce the run time while keeping sufficient accuracy in the computed irradiances that the resulting chlorophyll values remained within a few percent of the EcoLight baseline values. Figure 2 shows the results when EcoLight was called only every 4 or 6 hours, rather than every hour. We see that the results are almost unchanged even in the 6 hour runs, which took only 14% longer than the run with the inaccurate analytic irradiance model. Figure 3 shows the results when EcoLight is run at 5 (the baseline), 20, 50, and 100 nm wavelength resolution. Irradiances at uncomputed wavelengths were obtained by linear interpolation between the computed values. We see that 20 nm resolution is as good as 5, but that (not surprisingly) the results begin to differ at 50 nm resolution. Finally, Fig. 4 shows the results when the RTE is solved to different depths, with the uncomputed values at deeper depths being obtained by extrapolation of the deepest-computed value. We see that solving the RTE to about the

20% light level ($F = 0.2$) is adequate, and reduced the run time to only 17% more than the analytic calculations.

Figure 5 shows the results for a combination of the above EcoLight options, namely recomputing the irradiance *de novo* every 4 hours, at 25 nm resolution, and down to the 15% light level. The increase in run time for this EcoLight optimization is only 14% compared to the baseline run with the analytic light model, and the results differ by only a few percent from those obtained when EcoLight is called hourly, at 5 nm resolution, and down to the 0.1% light level. Figure 5 thus shows that ***if EcoLight is called intelligently*** (i.e., not at every grid point, not at every time step, not at every wavelength, etc.) within the ROMS-EcoSim model, ***EcoLight requires only slightly more computation time than the simple analytical model***. However, the irradiances computed by an optimized EcoLight calling scheme are still much more accurate than those computed by the baseline analytical model, and the significant differences in ecosystem predictions are preserved.

Figure 6 shows the *Chl* depth profiles of Chlorophyll at midsummer of year 5 for the baseline analytic (black and purple curves) and EcoLight runs (dark blue), for the optimized EcoLight run (green), and for two EcoLight runs that did not solve the RTE deep enough (red) or at enough wavelengths (aqua).

Finally, Fig. 7 shows the year 5 time series for the four phytoplankton functional groups whose total chlorophyll values are plotted in the previous figures. We see that the difference in the approximate and accurate irradiance calculations delays and magnifies the spring *synechococcus* bloom more than the other functional groups.

IMPACT/APPLICATION

Predictive ecosystem models are playing an increasingly important role in our understanding of the oceans. Applications of such models range from predictions of water clarity for military purposes to management of coastal waters for fisheries. The incorporation of the EcoLight model developed here into coupled ecosystem models will give improved accuracy in the predictions of primary production and related quantities made by such models. As the coupled models become more trustworthy in their predictions, they will become even more valuable as tools for ocean science and aquatic ecosystem management.

TRANSITIONS

A previous version of the EcoLight code was delivered to Dr. Paul Bissett of the Florida Environmental Research Institute (FERI). He used the code for various ecosystem studies, including hindcast simulations of the West Florida Shelf as reported in Bissett et al. (2008). A version of the EcoLight code will be bundled in the next version of HydroLight, which is now under development.

RELATED PROJECTS

This work is a collaboration between myself, Lydia Sundman of Sundman Consulting (EcoLight coding and BioToys simulations), Paul Bissett of FERI (assistance with EcoSim), and Bronwyn Cahill, a postdoctoral student at Rutgers University (assistance with ROMS). Their participation was supported by the present contract.

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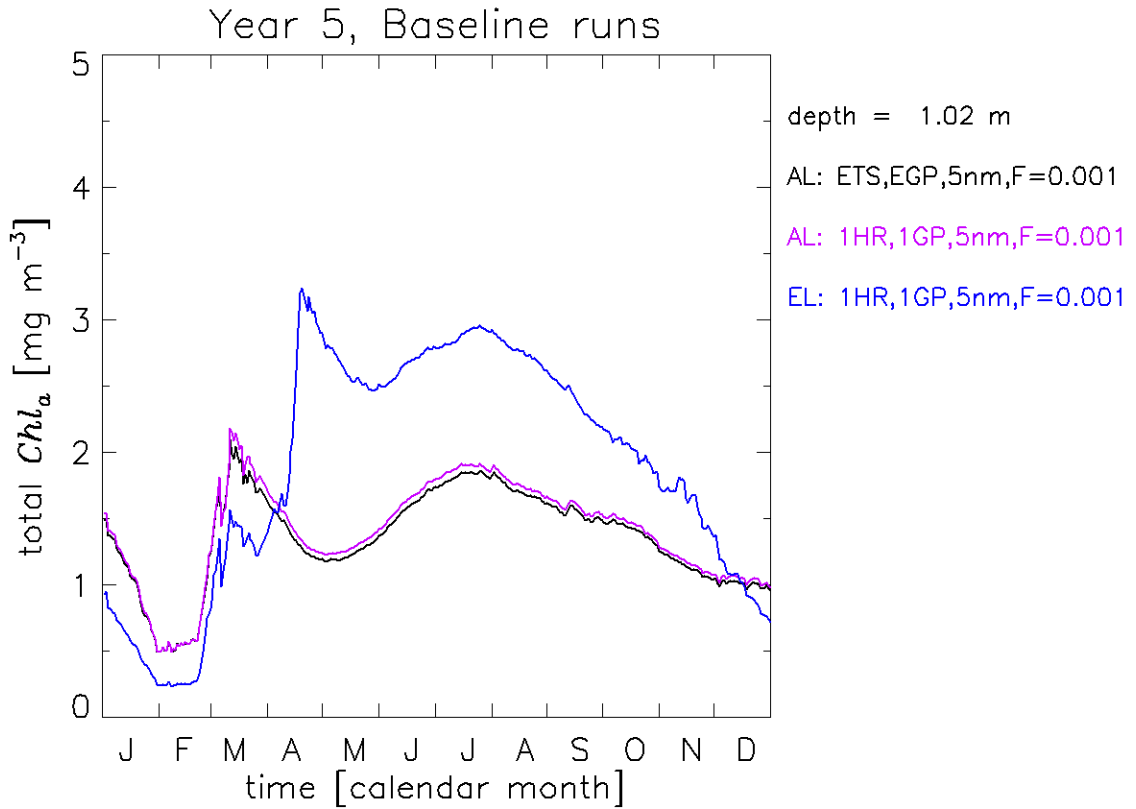


Fig. 1. The black line shows the BioToys near-surface total chlorophyll values during simulation year 5 when using the default BioToys analytic irradiance model (AL) with the irradiances being updated every 9 minutes at every grid point. The purple curve show the results when irradiances are updated ever hour at one grid point. The difference in these two runs is less that 2%. The blue curve shows the results when EcoSim's approximate analytic irradiance model is replaced by EcoLight (EL), with EcoLight being called every hour at one grid point. The difference is now as much as a factor of two in magnitude, and over a month in the time of the spring bloom. [The figure color codes the plotted chlorophyll a time series.]

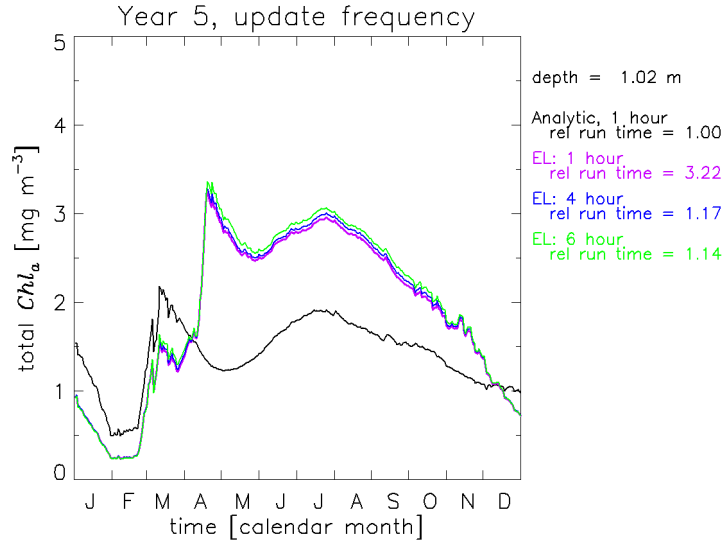


Fig. 2. Comparison of runs with *Ecolight* being called hourly, or every 4 or 6 hours, to recompute the irradiances. “rel run time” gives the total run time relative to the time needed by the analytic irradiance model.

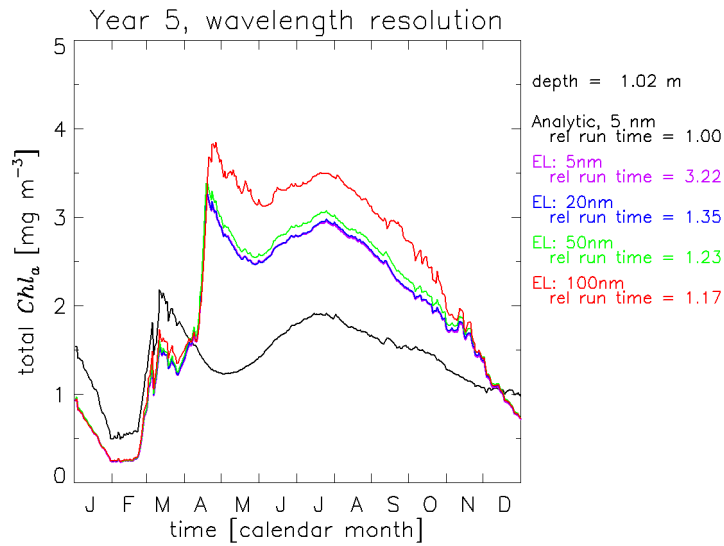


Fig. 3. Comparison of runs with *Ecolight* computing the spectral irradiance at different wavelength resolutions. The black curve is the analytic light model, the purple curve is the baseline *EcoLight* model, and the other colors are various wavelength resolutions in the *EcoLight* runs.

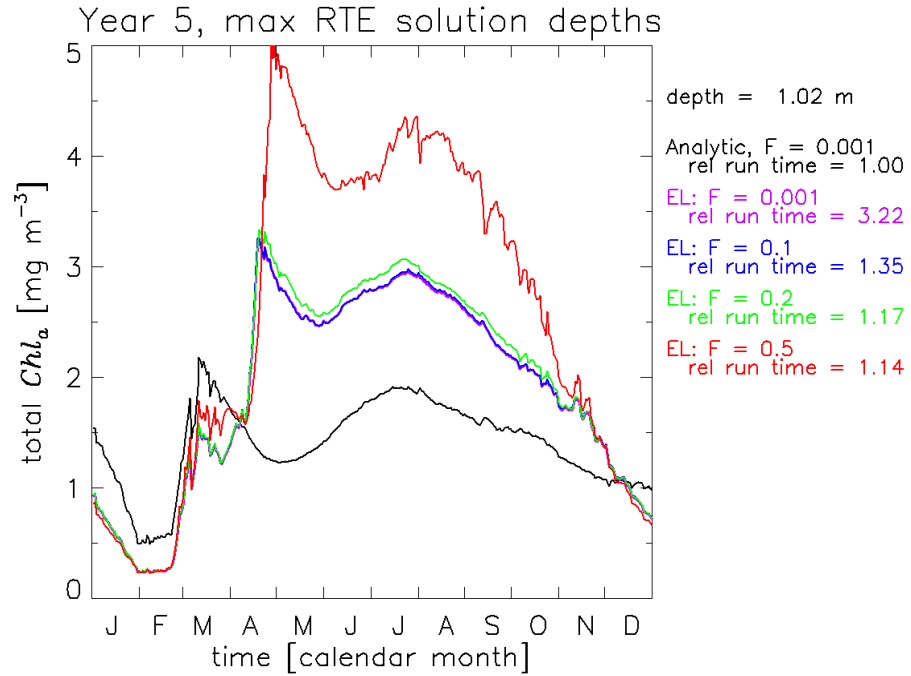


Fig. 4. Comparison of runs with Ecolight solving the RTE to different depths.

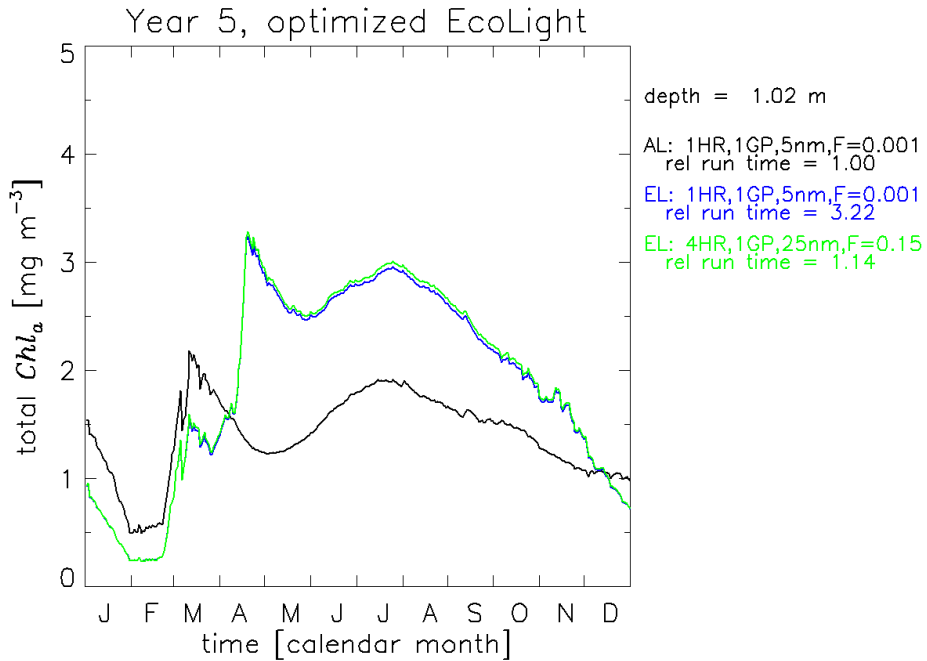


Fig. 5. Comparison of analytic and EcoLight base runs with an optimized EcoLight run that required only 14% more computation time than the analytic model, but which gave almost exactly the same chlorophyll values as the baseline EcoLight run.

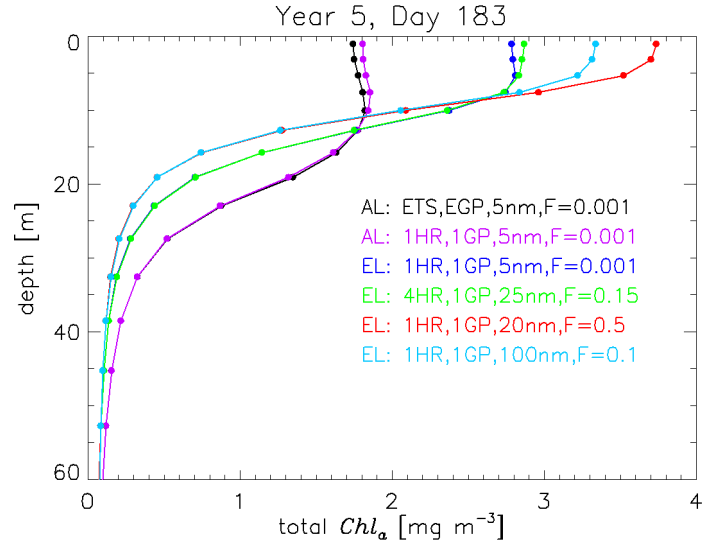


Fig. 6. Comparison of depth profiles of Chlorophyll at midsummer of year 5 for the baseline analytic (black and purple curves) and EcoLight runs (dark blue), for a well-optimized EcoLight run (green), and for two EcoLight runs that did not solve the RTE deep enough (red) or at enough wavelengths (aqua).

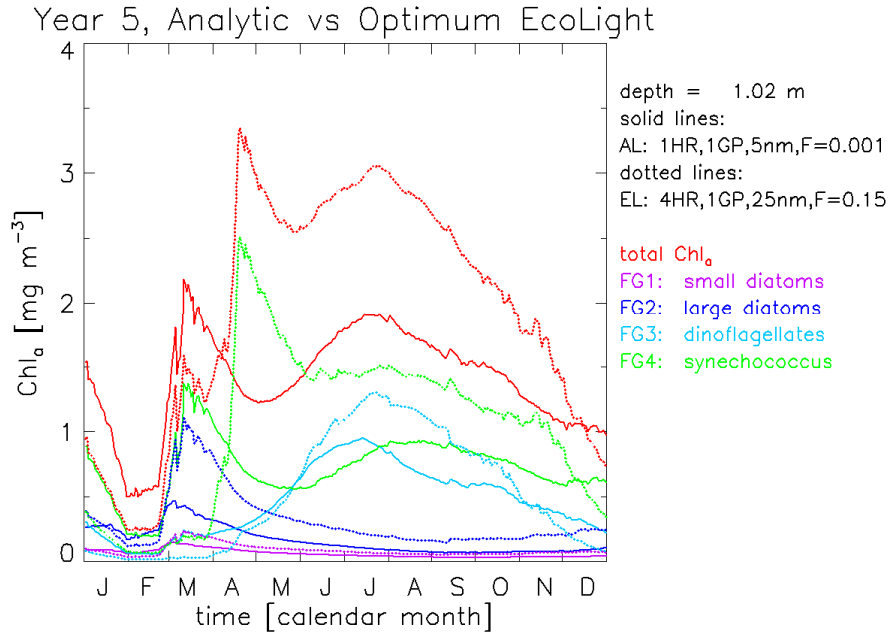


Fig. 7. Comparison of phytoplankton functional groups for the analytic and the optimized EcoLight run of Fig. 5, which required only 14% more computation time than the analytic model but which gave almost exactly the same chlorophyll values as the baseline EcoLight run. Note that the onset of the synechococcus spring bloom is much different in these two runs, whereas the diatoms and

dinoflagellates bloom at the same times, but with different magnitudes.